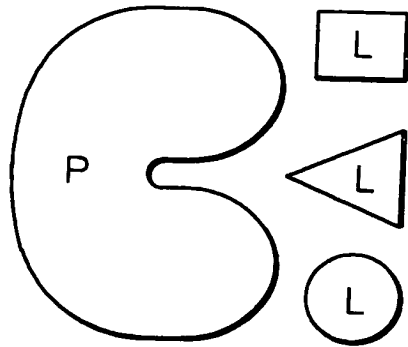


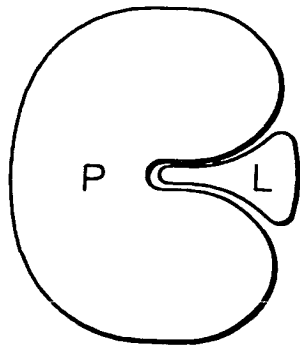
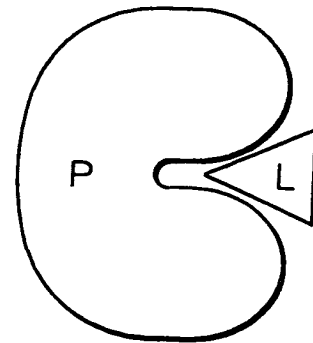
Patented 3342260

APPROVED BY DRAFTSMAN	O.G. FIG.	
	CLASS	SUBCLASS



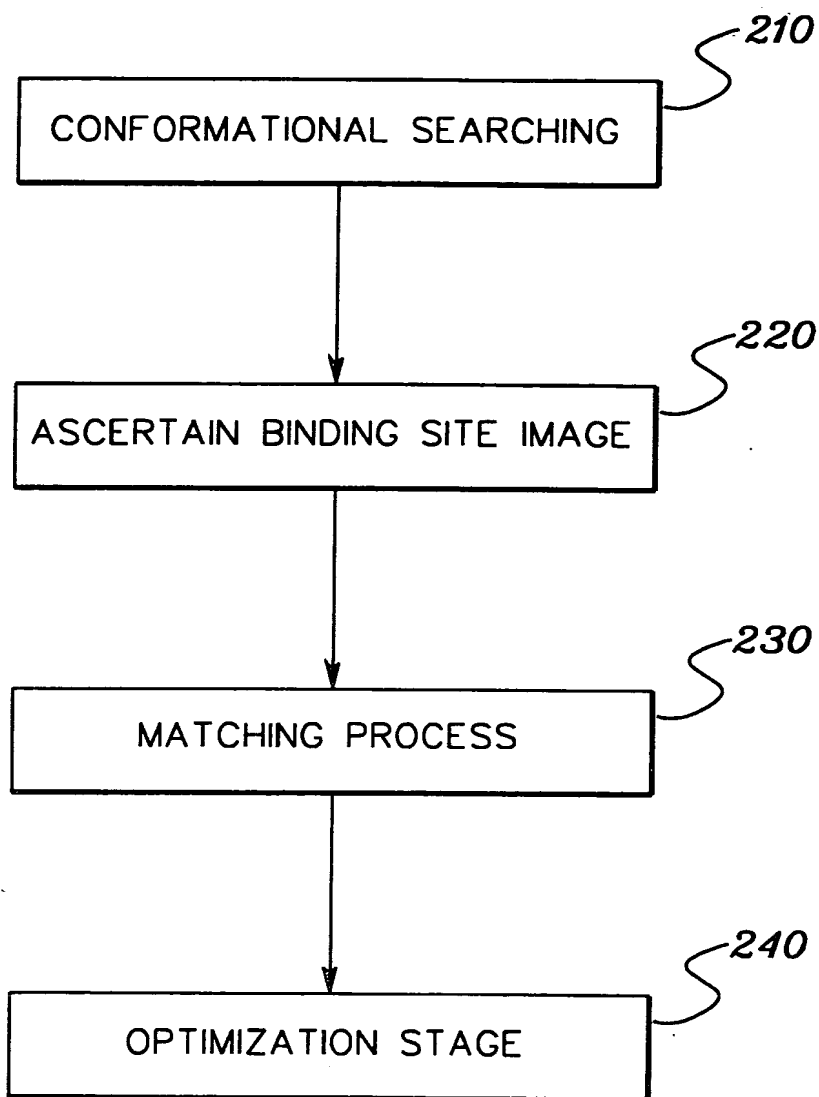
*fig. 1A*

*fig. 1B*



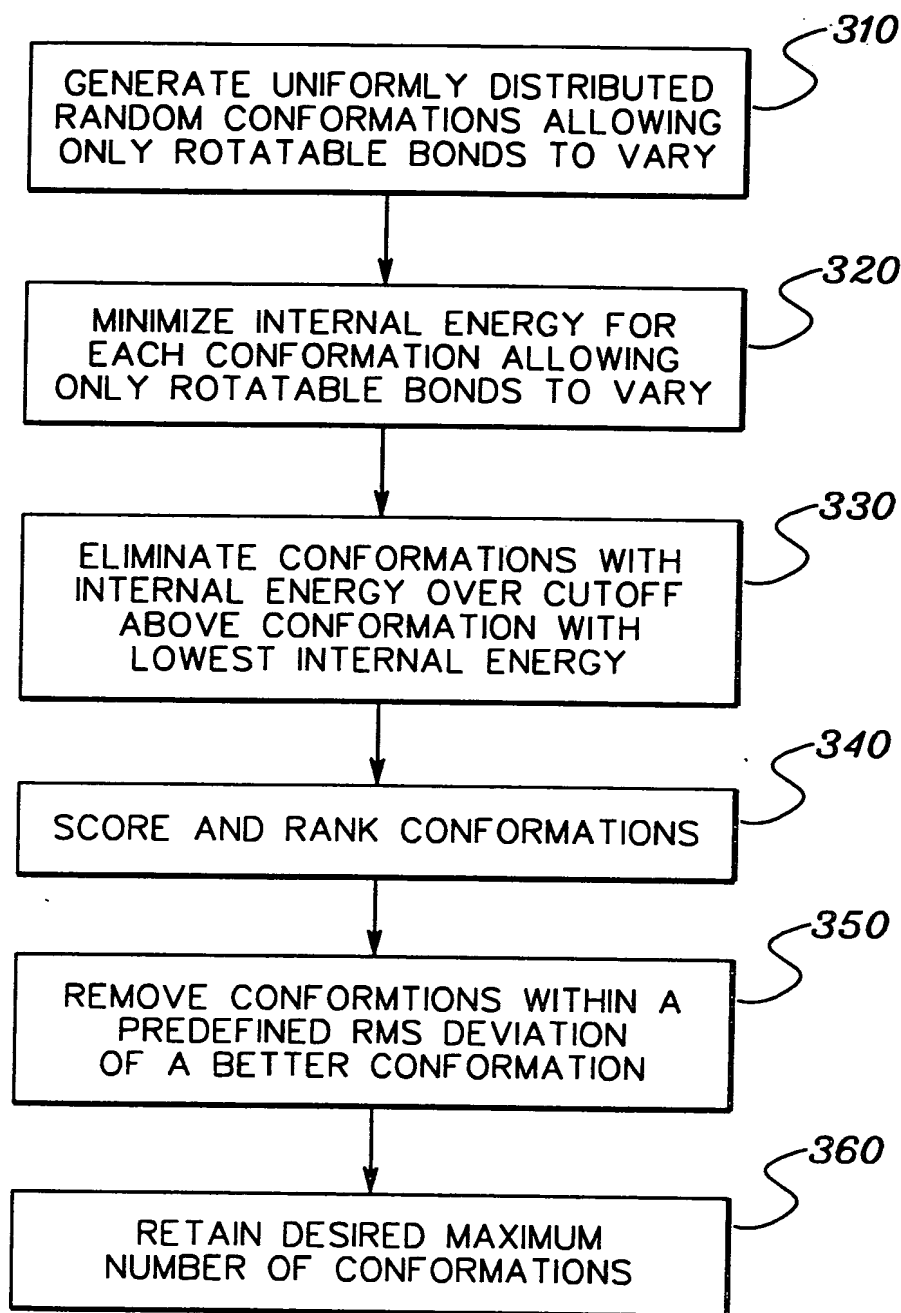
*fig. 1C*

APPROVED BY DRAFTSMAN	O.G. FIG.	
	CLASS	SUBCLASS



*fig. 2*

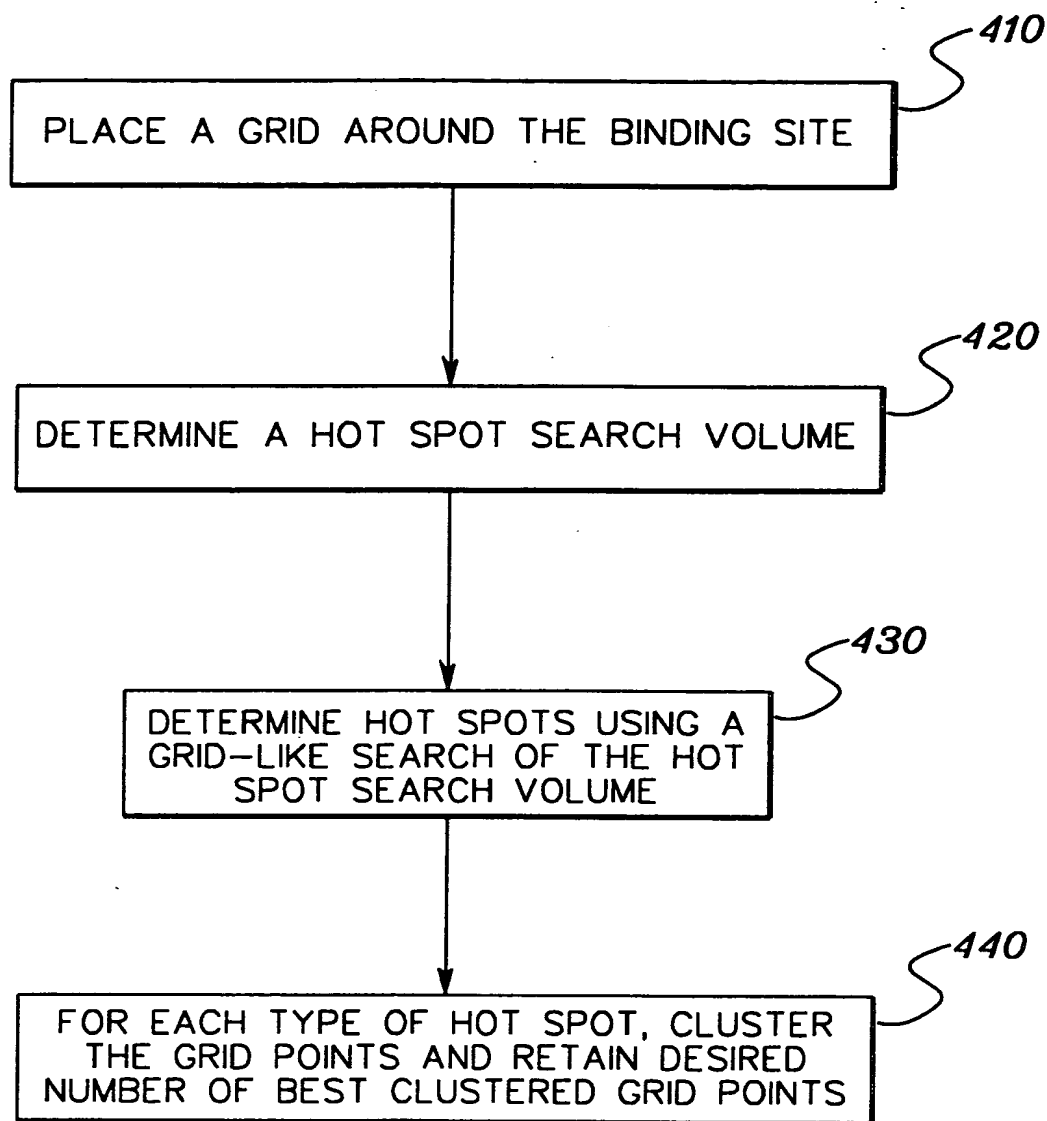
O.G. FIG.	
APPROVED BY	DRAFTSMAN
CLASS	SUBCLASS



*fig. 3*

O.G. FIG.		SUBCLASS
APPROVED	BY	DRAFTSMAN

FIG. 4 is a flow diagram



*fig. 4*

APPROVED BY DRAFTSMAN	O.G. FIG.	
	CLASS	SUBCLASS

INITIALLY MATCH THE ATOMS OF A LIGAND  
TO THE APPROPRIATE HOT SPOTS

USE EACH MATCH TO DETERMINE A UNIQUE RIGID  
BODY TRANSFORMATION THAT MINIMIZES

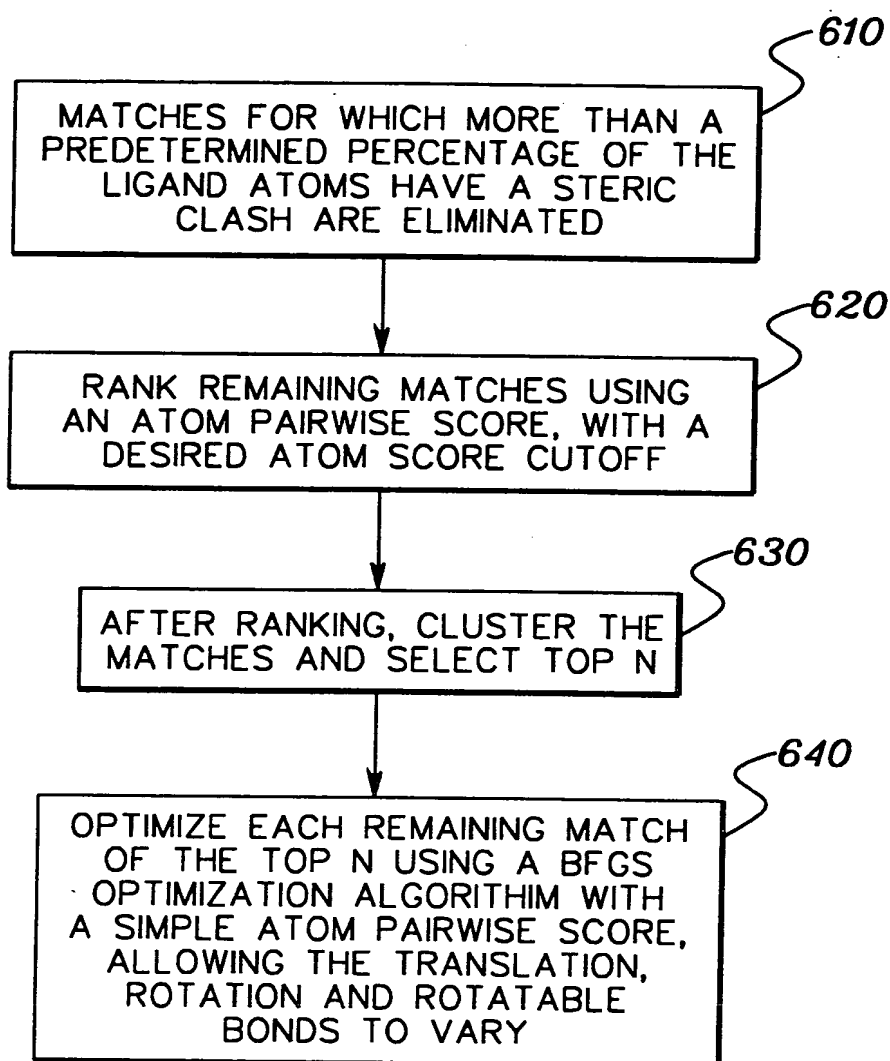
$$I(R.T) = \sum_{j=1}^3 |H_j - RA_j - T|^2$$

USE EACH UNIQUE RIGID BODY TRANSFORMATION  
TO PLACE THE LIGAND CONFORMATION  
INTO THE BINDING SITE

*fig. 5*

APPROVED BY DRAFTSMAN	O.G. FIG.	SUBCLASS
	CLASS	

Patented 2000



*fig. 6*

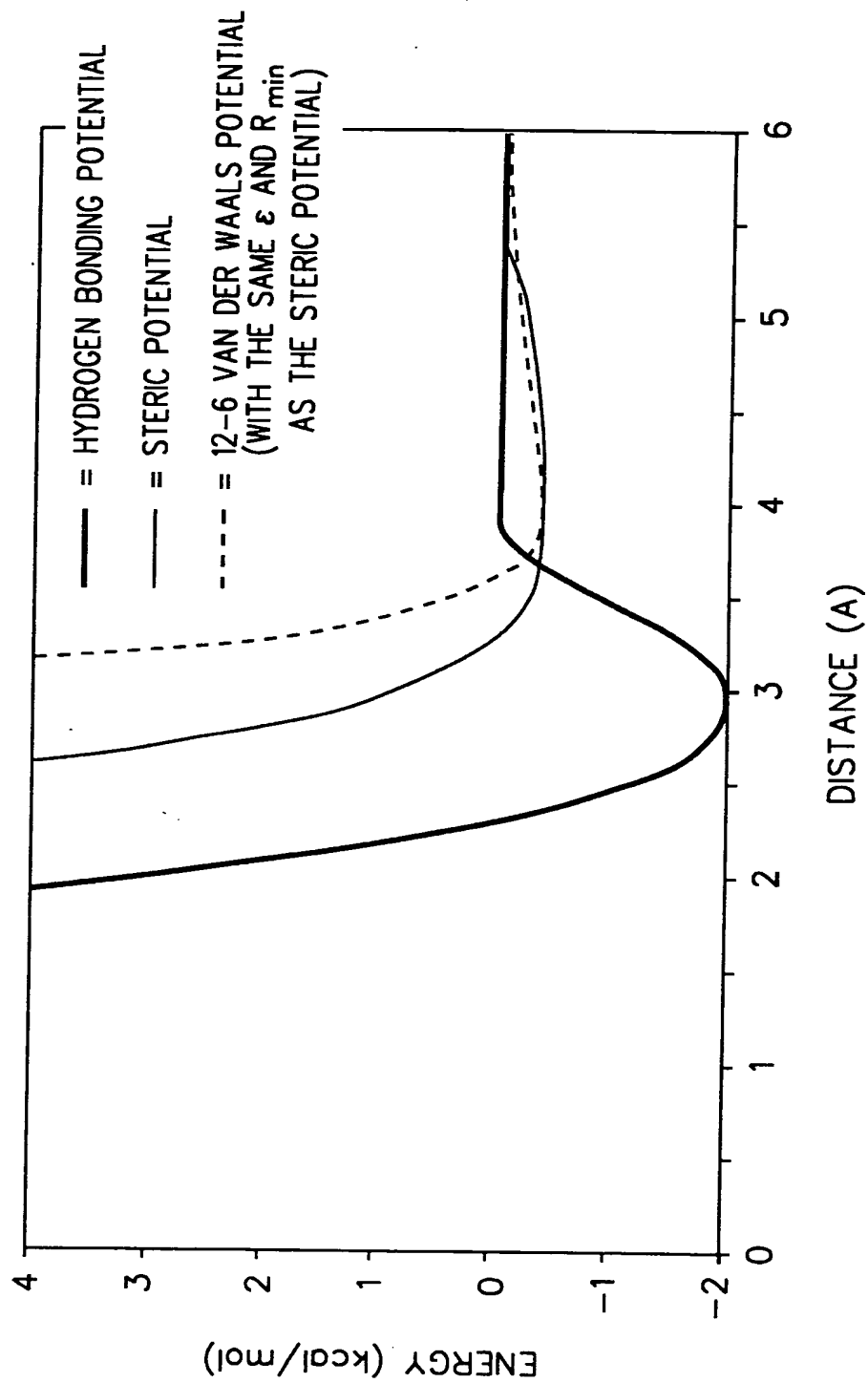
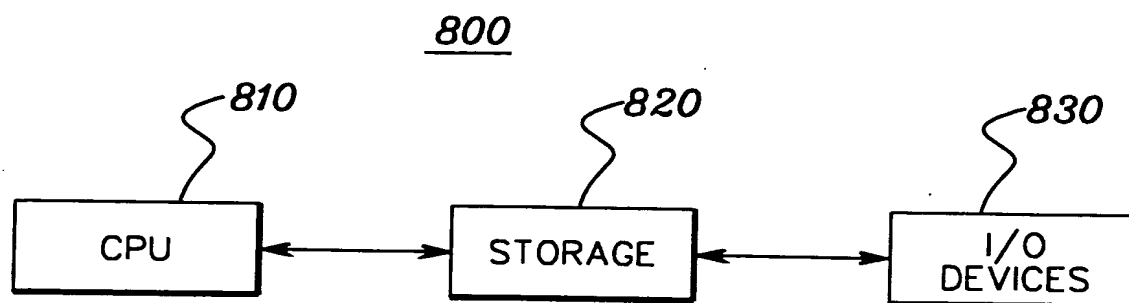


fig. 7

APPROVED BY DRAFTSMAN	O.G. FIG.	
	CLASS	SUBCLASS



*fig. 8*



FIG. 9

APPROVED	O.G. FIG.	
BY	CLASS	SUBCLASS
DRAFTSMAN		

9/10

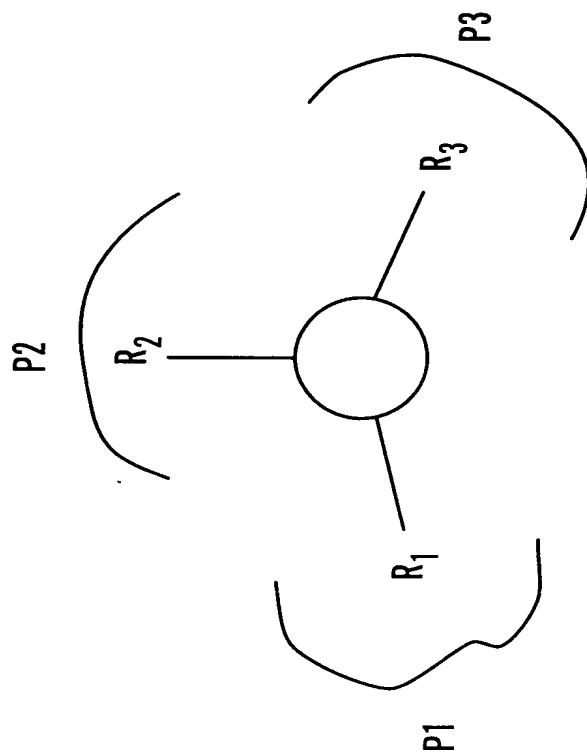


FIG. 9

APPROVED BY DRAFTSMAN	O.G. FIG.	
	CLASS	SUBCLASS

10/10

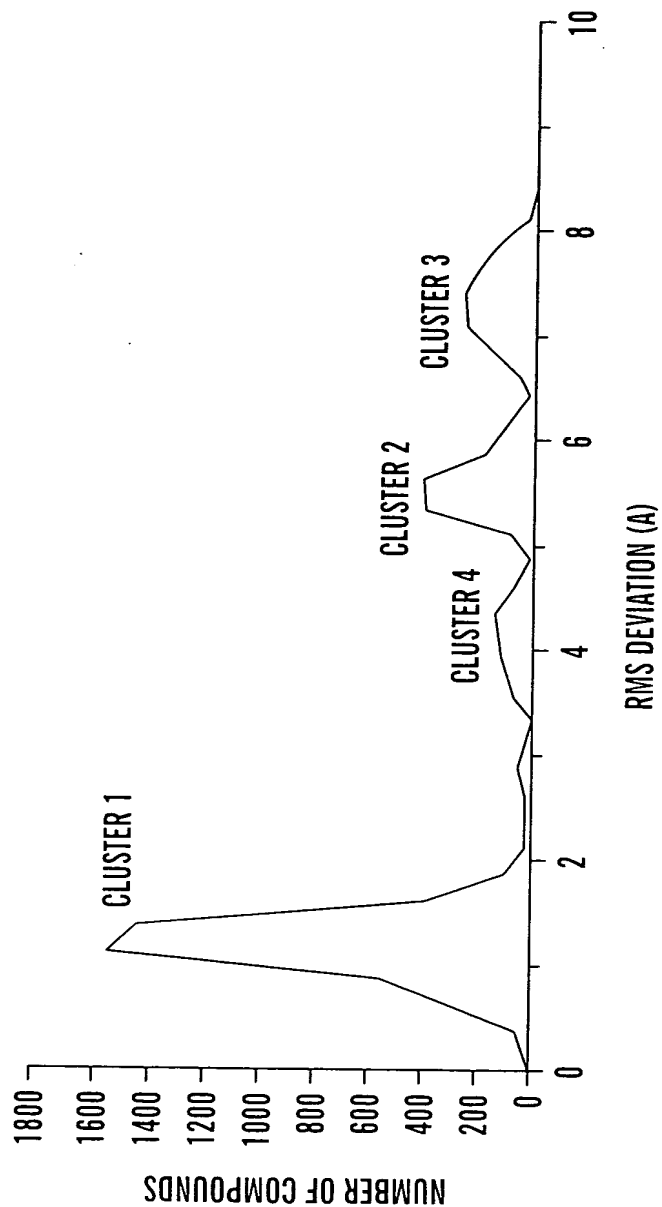


FIG. 10